Application of Computational Materials Science Multiscale Modeling to Fission Reactors

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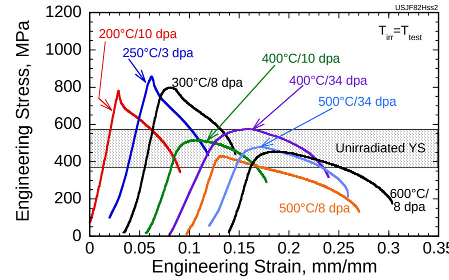
Workshop on Advanced Simulations: A Critical Tool for Future Nuclear Fuel Cycles

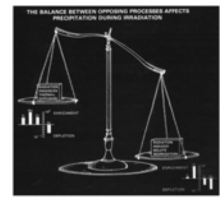
Lawrence Livermore National Laboratory, December 14-16, 2005

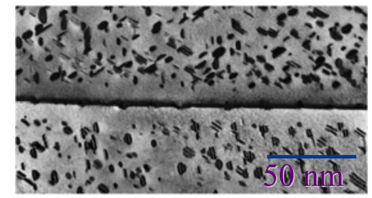
Radiation Damage can Produce Large Changes in Structural Materials

- **Radiation hardening and embrittlement ($<0.4\ T_M$, >0.1 dpa)**



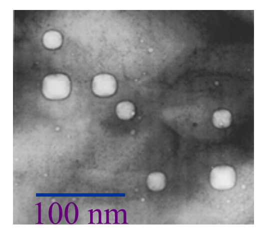
- **Phase instabilities from radiation-induced precipitation (0.3-$0.6\ T_M$, >10 dpa)**

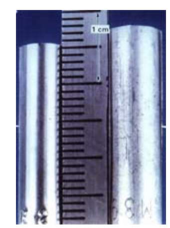




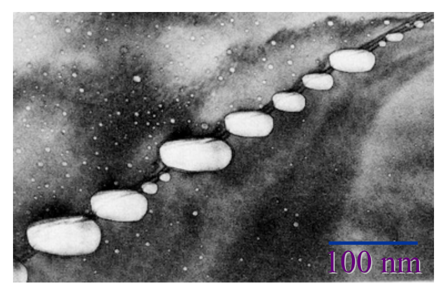
- **Irradiation creep ($<0.45\ T_M$, >10 dpa)**

- **Volumetric swelling from void formation (0.3-$0.6\ T_M$, >10 dpa)**





- **High temperature He embrittlement ($>0.5\ T_M$, >10 dpa)**



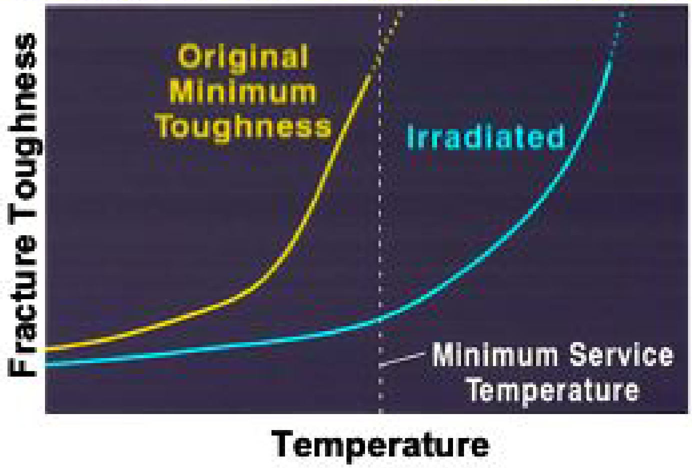
Comparison of fission and fusion structural materials requirements

	Fission (Gen. I)	Fission (Gen. IV)	Fusion (Demo)	NASA space react.
Structural alloy maximum temperature	<300˚C	500-1000˚C	550-1000˚C	~1000˚C
Max dose for core internal structures	~1 dpa	~30-100 dpa	~150 dpa	~10 dpa
Max transmutation helium concentration	~0.1 appm	~3-10 appm	~1500 appm (~10000 appm for SiC)	~1 appm
Coolants	H_2O	He, H_2O, Pb-Bi, Na	He, Pb-Li, Li	Li, Na, or He-Xe
Structural Materials	Zircaloy, stainless steel	Ferritic steel, SS, superalloys, C- composite	Ferritic/ martensitic steel, V alloy, SiC composite	Nb-1Zr, Ta alloys, Mo alloys, superalloys

- Common theme for fusion,Gen IV fission and space reactors is the need to develop higher temperature materials with adequate radiation resistance

Understanding the Effects of Irradiation on Structural Materials Requires Multiscale Modeling (and Experiments)

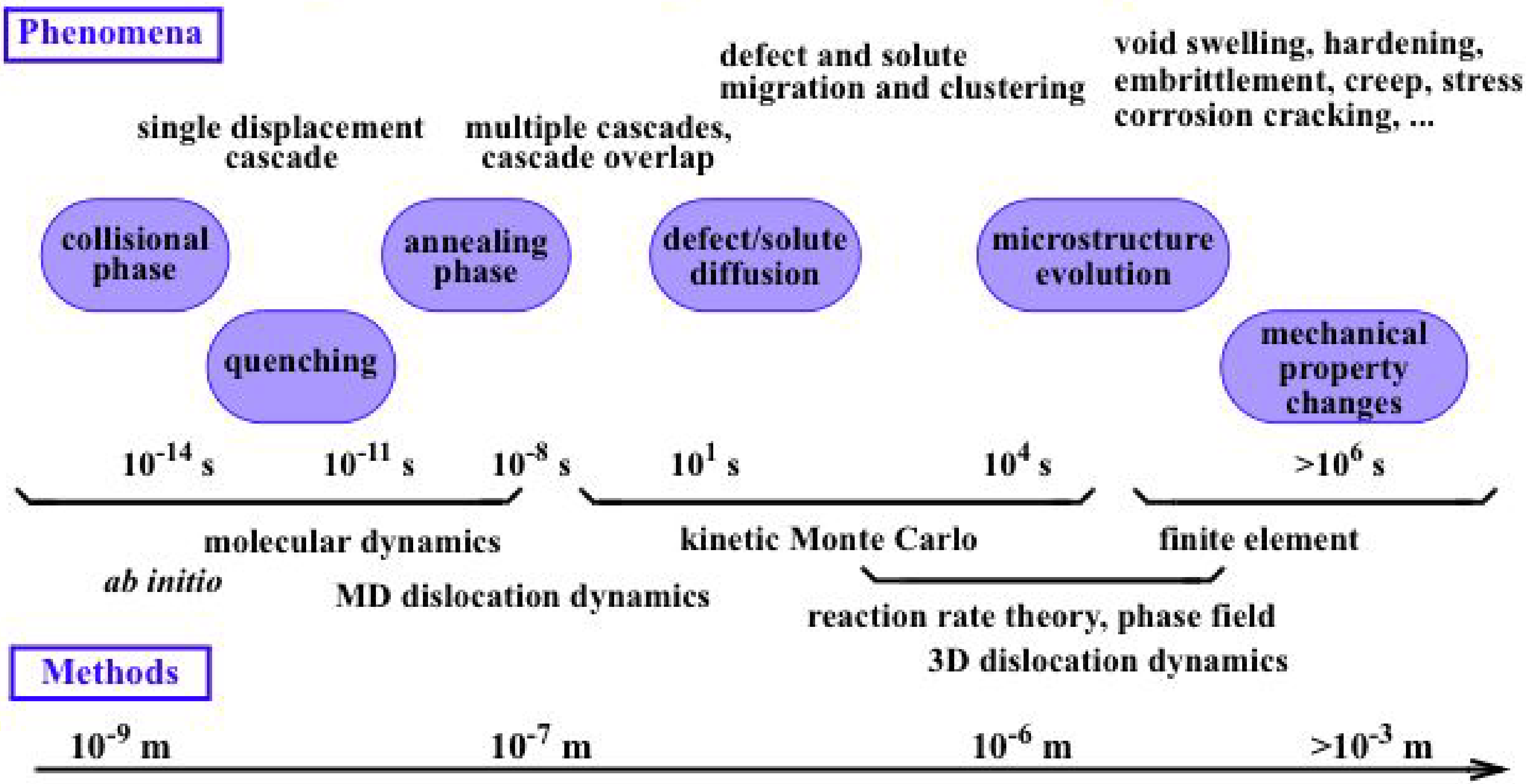
- critical fracture toughness of 800 ton reactor pressure vessel can be severely degraded by radiation-induced defect structure on the size scale of 2 to 3 nm



- copper and manganese-enriched clusters in neutron irradiated model RPV steel, APFIM data

R.E. Stoller

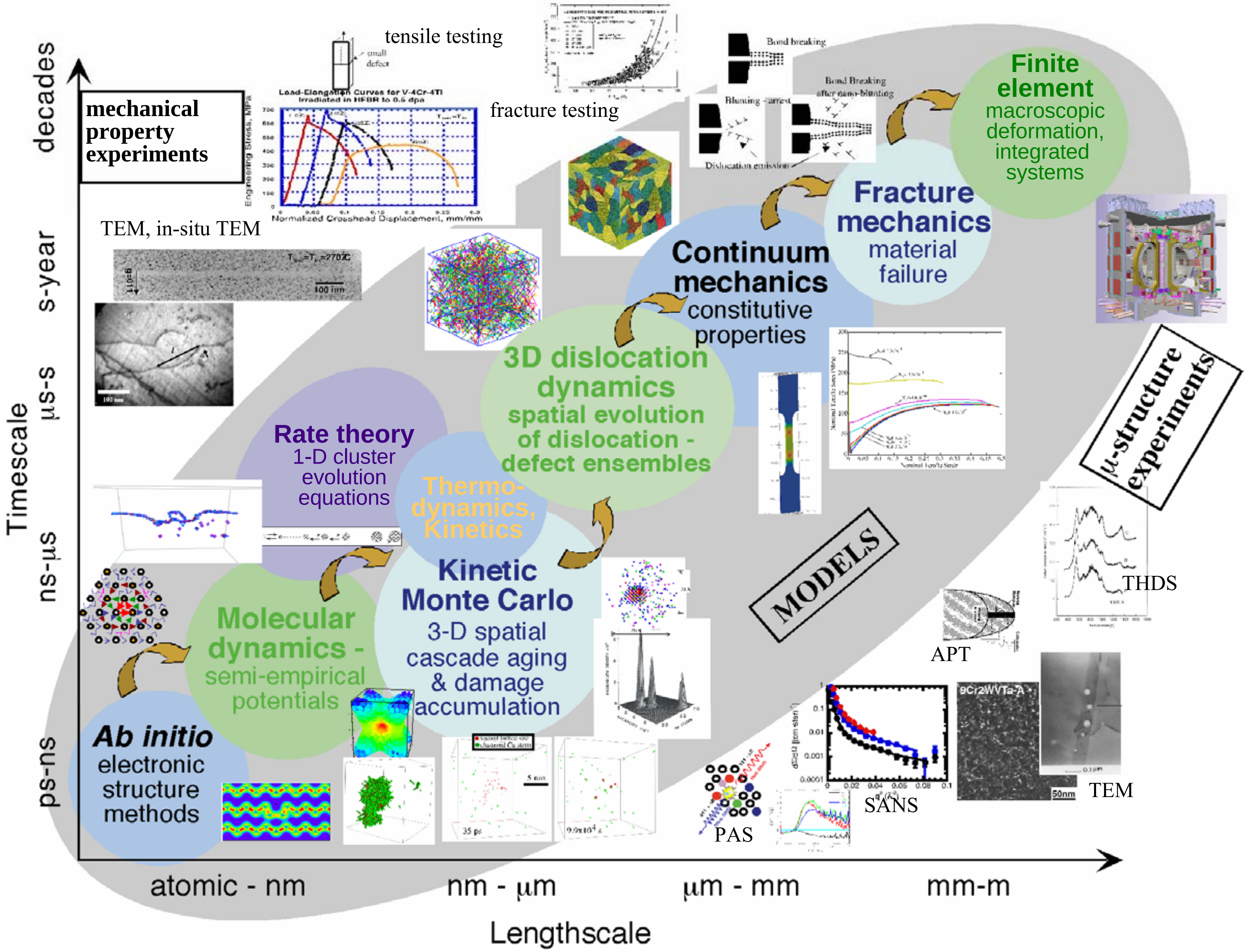
Schematic diagram: relevant phenomena and computational methods



Goal of multiscale modeling is fully predictive capability, but: "Prediction is very difficult, especially if it's about the future." ... Niels Bohr

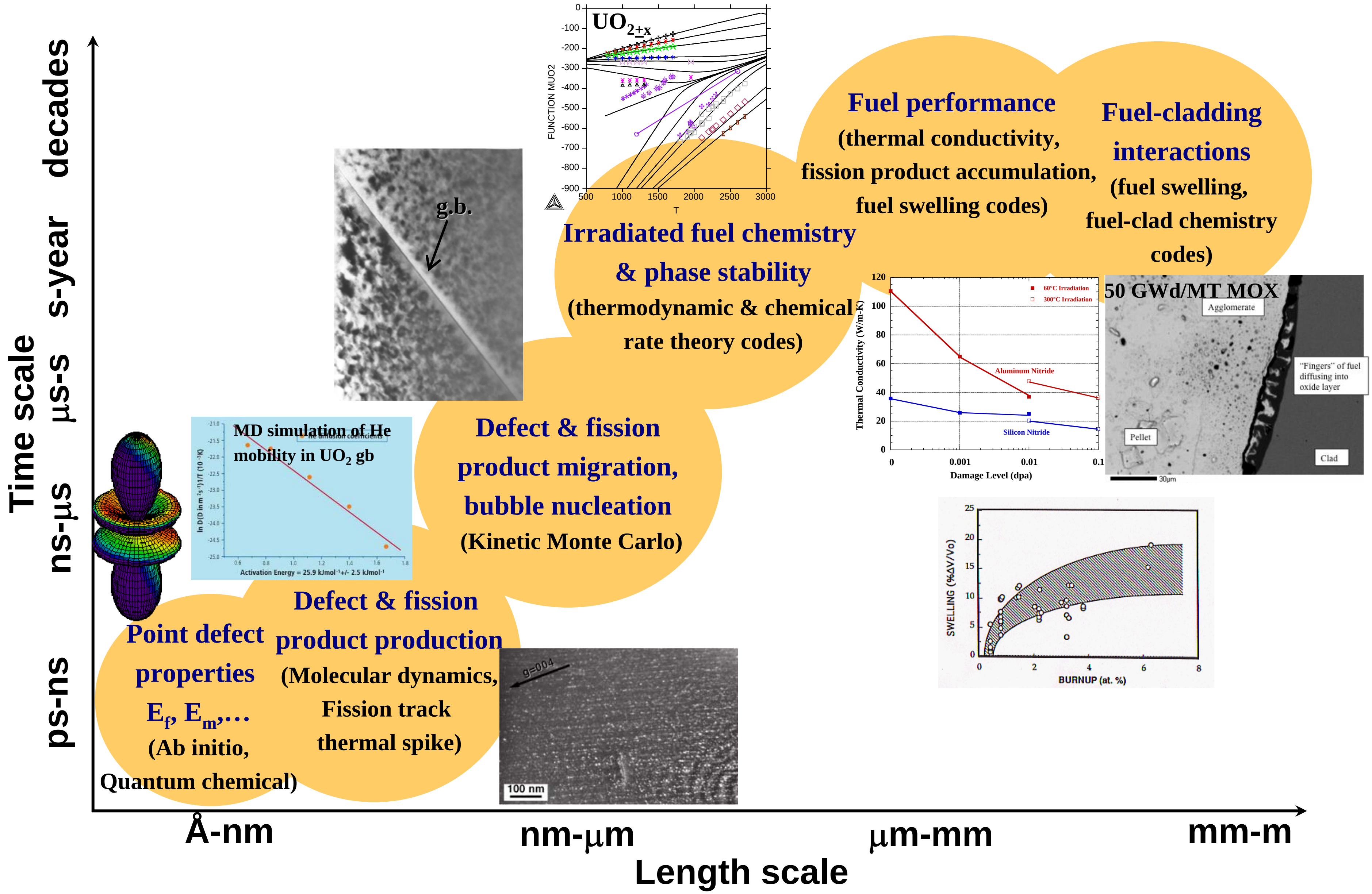
R.E. Stoller

Radiation damage is inherently multiscale with interacting phenomena ranging from ps to decades and nm to m



B.D. Wirth, UC-Berkeley

Fission reactor fuels modeling is multiscale with similar interacting phenomena time and length scales as irradiated structural materials



Current status of 1st principles computational materials science*

- **Goal is to solve the Schrödinger equation (or Dirac eqn, if relativistic effects are important)**
  - **Trivial for hydrogen; very complex for higher mass systems due to many-body effects in the Hamiltonian**
  - **Electrons can be decoupled from ions using adiabatic approximation**
  - **Reducing the many-electron problem to an effective one-electron system requires approximations that can introduce significant errors**
- **Current "standard model" for condensed mater physics is Density Functional Theory (DFT) using Local Density Approximation (LDA)**
  - **Currently limited to 100-1000 atoms (n^3 scaling)**
    - **Largest MD-DFT simulation to date (2004) is 1080 B atoms (n=3840 electrons) on LLNL's 2000 CPU Linux cluster**
    - **Need to accurately model behavior of ~10^{12} to 10^{15} atoms (Z~25) to simulate behavior occurring within one individual grain**
  - **Generally successful in predicting structures and macroscopic properties**
  - **Underpredicts band gap energies, overpredicts lattice parameters, predicts wrong ground state for some magnetic systems (e.g., Fe)**
  - **Generalized gradient approximation (GGA) in DFT fixes some of these errors but introduces other errors**
- **Quantum chemistry models provide best accuracy, but are computationally expensive (e.g., n^6 scaling)**

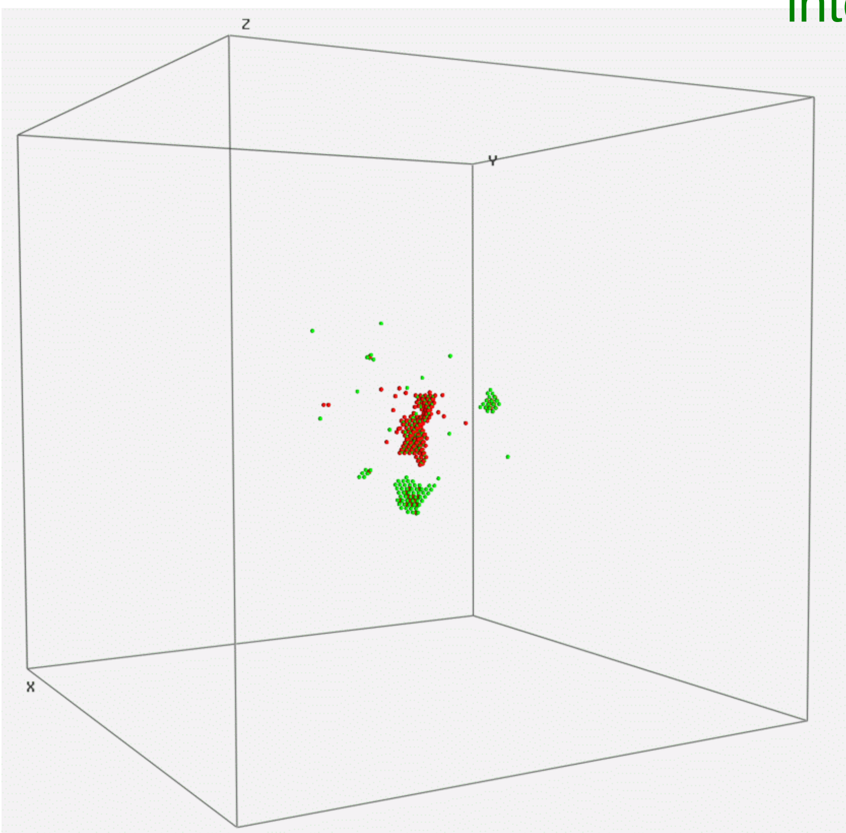
***Workshop on Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors, Washington DC, March 31-April 2, 2004,** http://www.csm.ornl.gov/meetings/SCNEworkshop/

Summary of DC modeling workshop: comparison with ASCI and DARPA AIM programs http://www.csm.ornl.gov/meetings/SCNEworkshop/

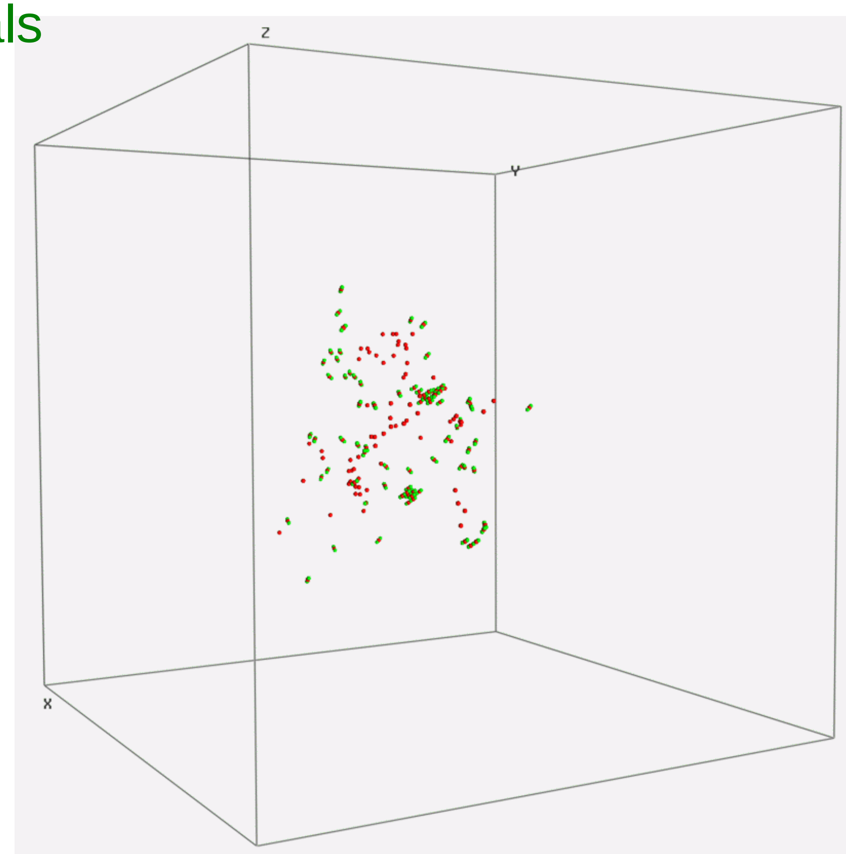
- **Even if sufficiently powerful supercomputers were available, there is still a strong need for experimental validation of model predictions (ASCI experience)**
  - **"…questionable whether [computational materials] science will be sufficiently mature in the foreseeable future to provide a rigorous scientific basis for predicting critical materials' properties, or for extrapolating well beyond the available validation database."**
- **The ASCI program encountered several challenges on the path to success, and the materials science community can and should learn from the ASCI experience**
  - **failing to account for the differences in code development paradigms as one scales from small code groups of a few staff developing a code with only a few major effects to a large group (20 or more) developing a multi-effect code**
  - **milestones were much too optimistic**
  - **Validation and verification are essential**

Comparison of surviving defects in a 25 keV displacement cascade in FCC (Cu) and BCC (Fe) metals

Vacancies
interstitials



Cu

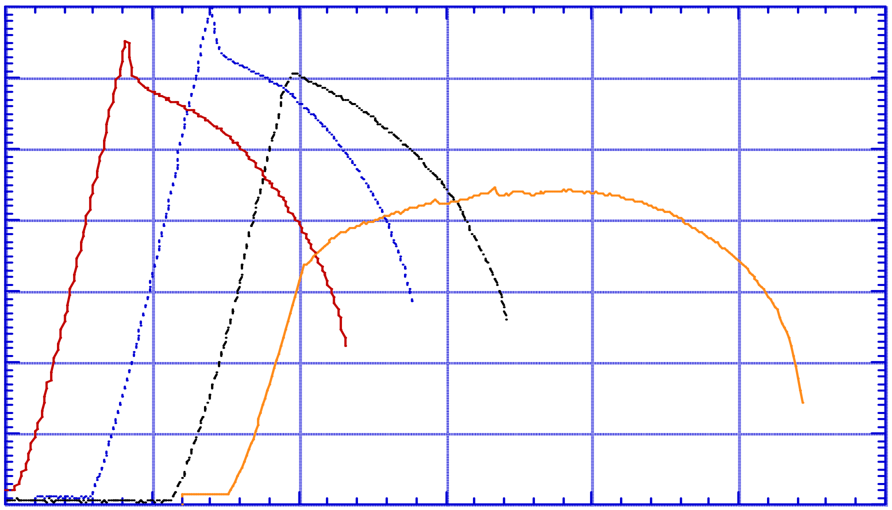


Fe

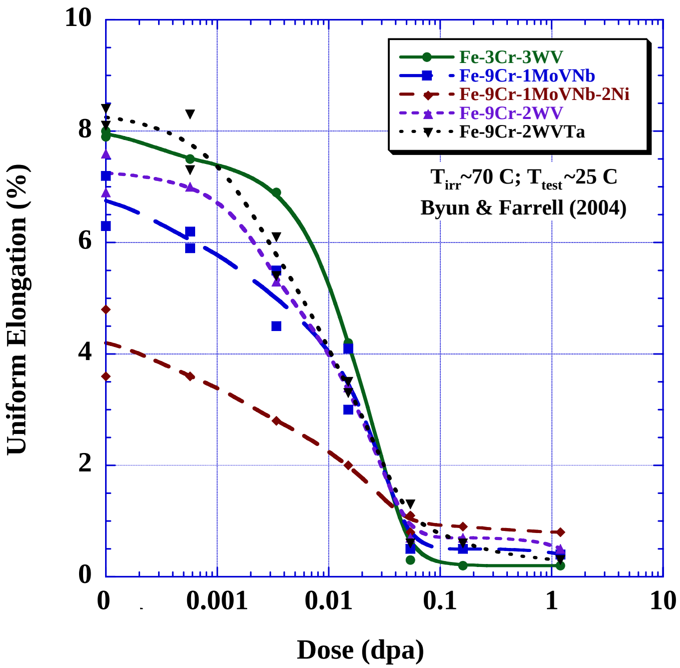
• Large vacancy clusters are not directly formed in BCC metal displacement cascades

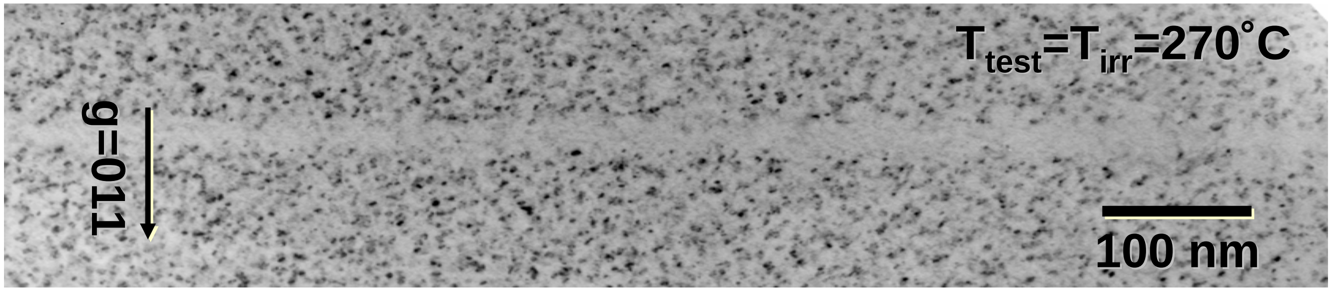
Yu. N. Osetsky and R.E. Stoller

Irradiated Materials Suffer Plastic Instability (due to Dislocation Channeling?)

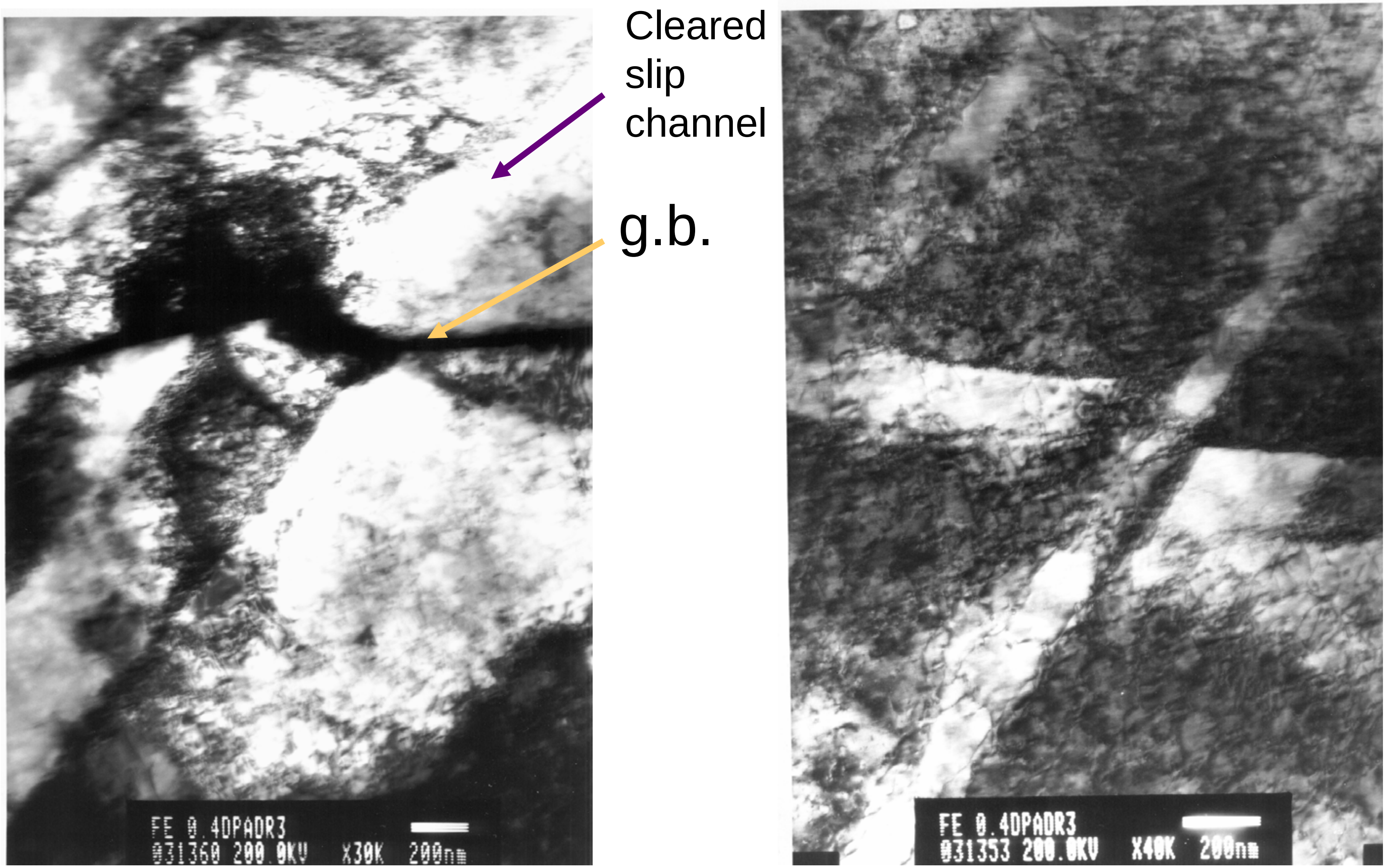


Effect of neutron irradiation on the uniform elongation of bainitic and ferritic/martensitic steels





Dislocation channel interactions in Fe deformed following neutron irradiation at 70˚C to 0.8 dpa



Need well-engineered materials to mitigate neutron radiation effects

Effect of temperature on edge dislocation interaction with 136 vacancy SFT in Cu

300 K

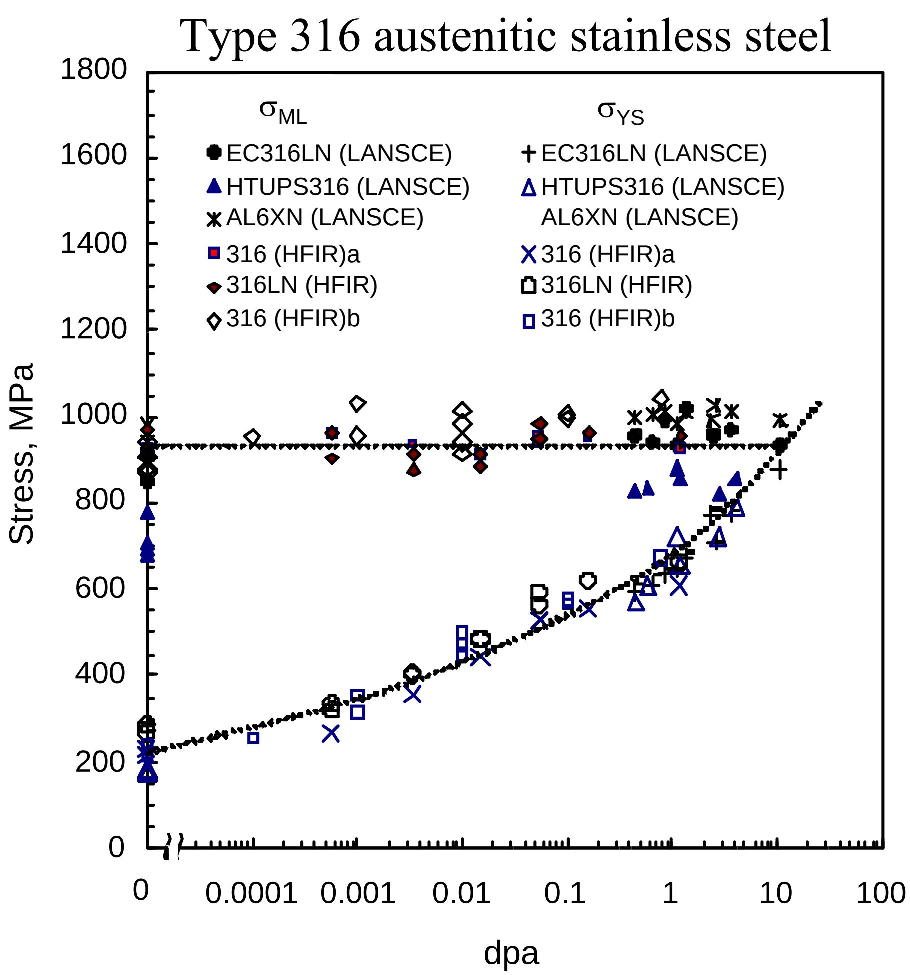
QuickTime™ and a
PNG decompressor
are needed to see this picture.

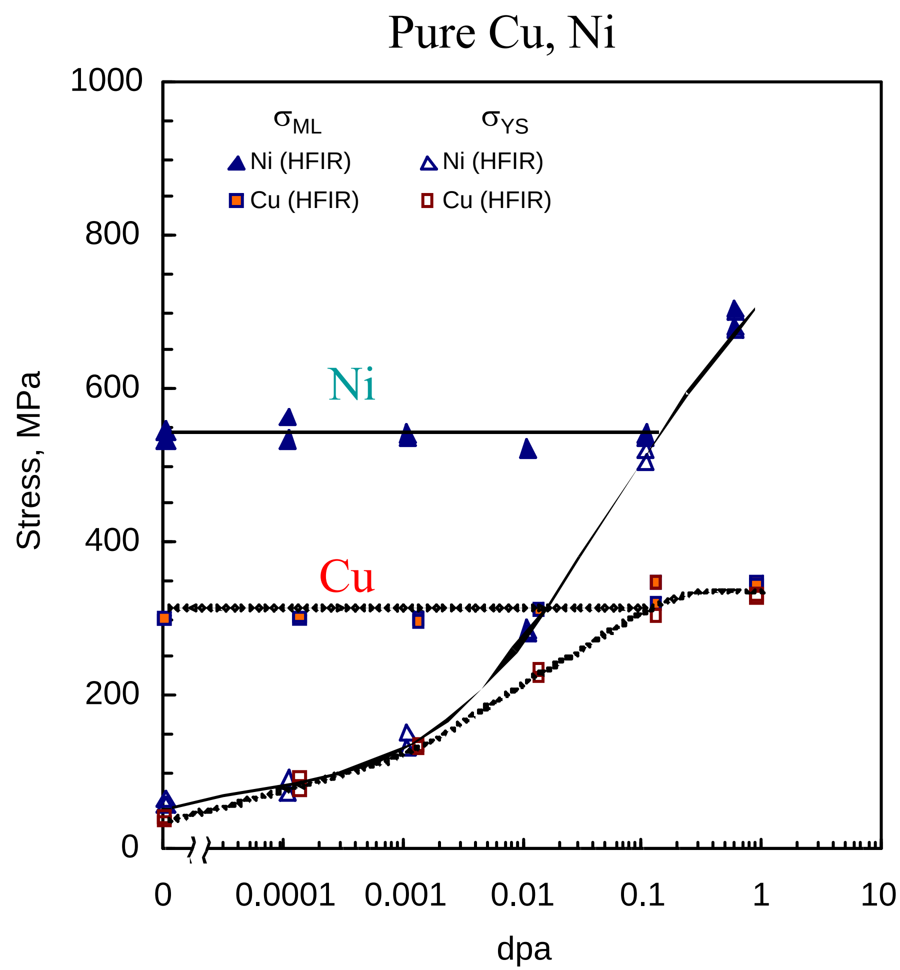
450 K

Defect cluster annihilation is enhanced at higher temperatures and slower strain rates (strain rate effect not shown)

- agrees with experimental results

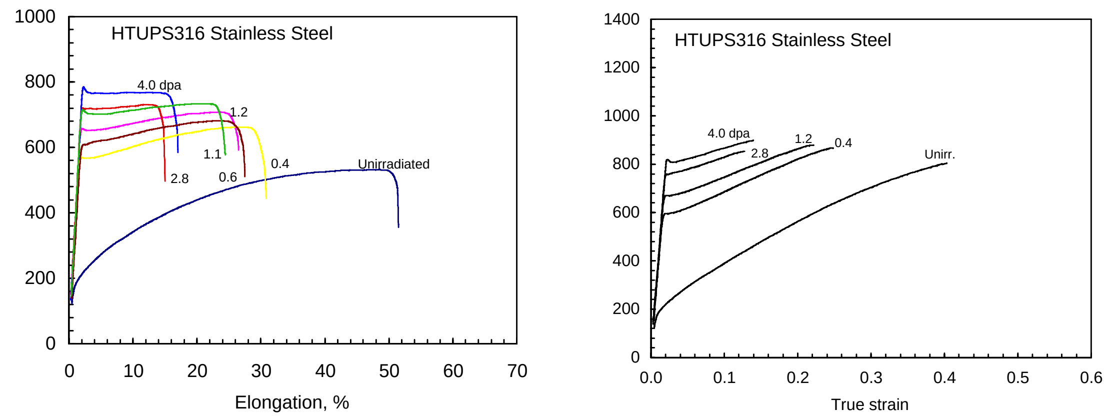
Plastic Instability Stress (σ_{PI}) of FCC Metals irradiated near 70°C





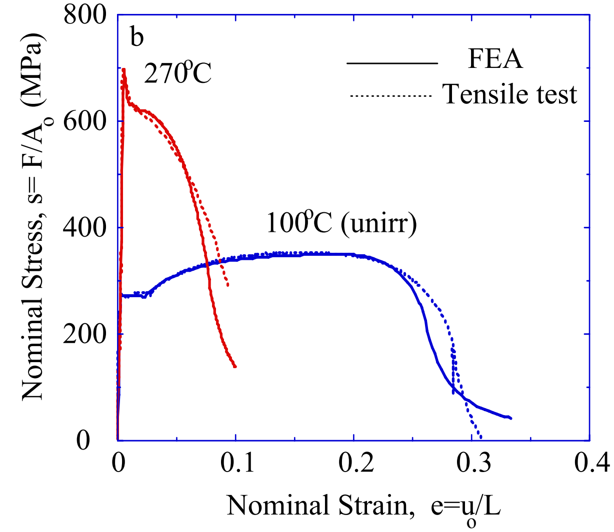
T.S. Byun & K. Farrell,
Acta Mater. 52 (2004) 1597

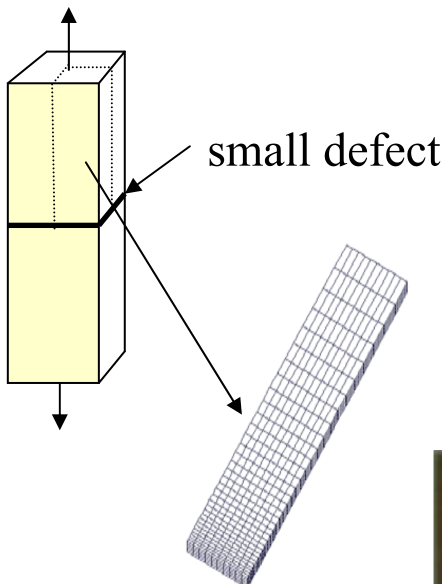
Understanding Loss of Uniform Strain Capacity

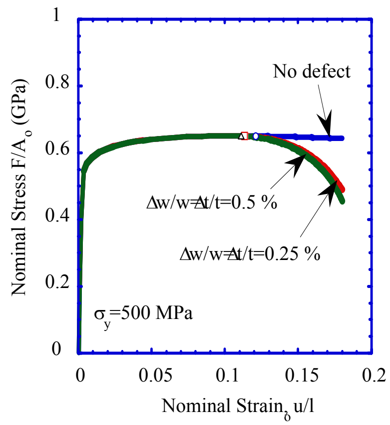


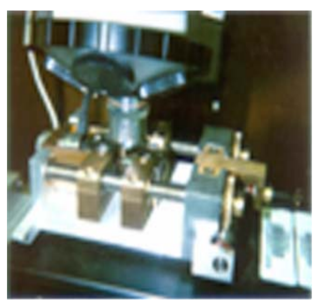
T.S. Byun et al., J. Nucl. Mater. 298 (2001) 269

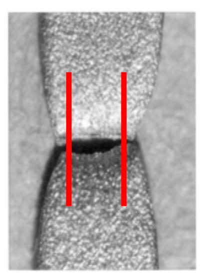
ABAQUS 1320 8-noded brick elements on 4x1x0.2 1/8 symmetry plate using J_2 incremental flow theory

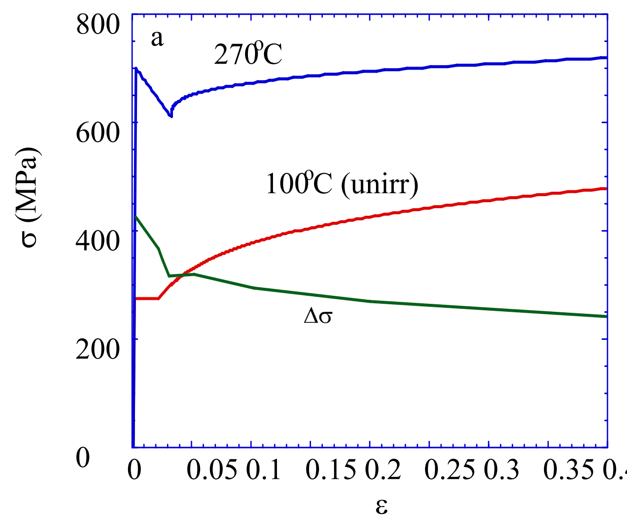








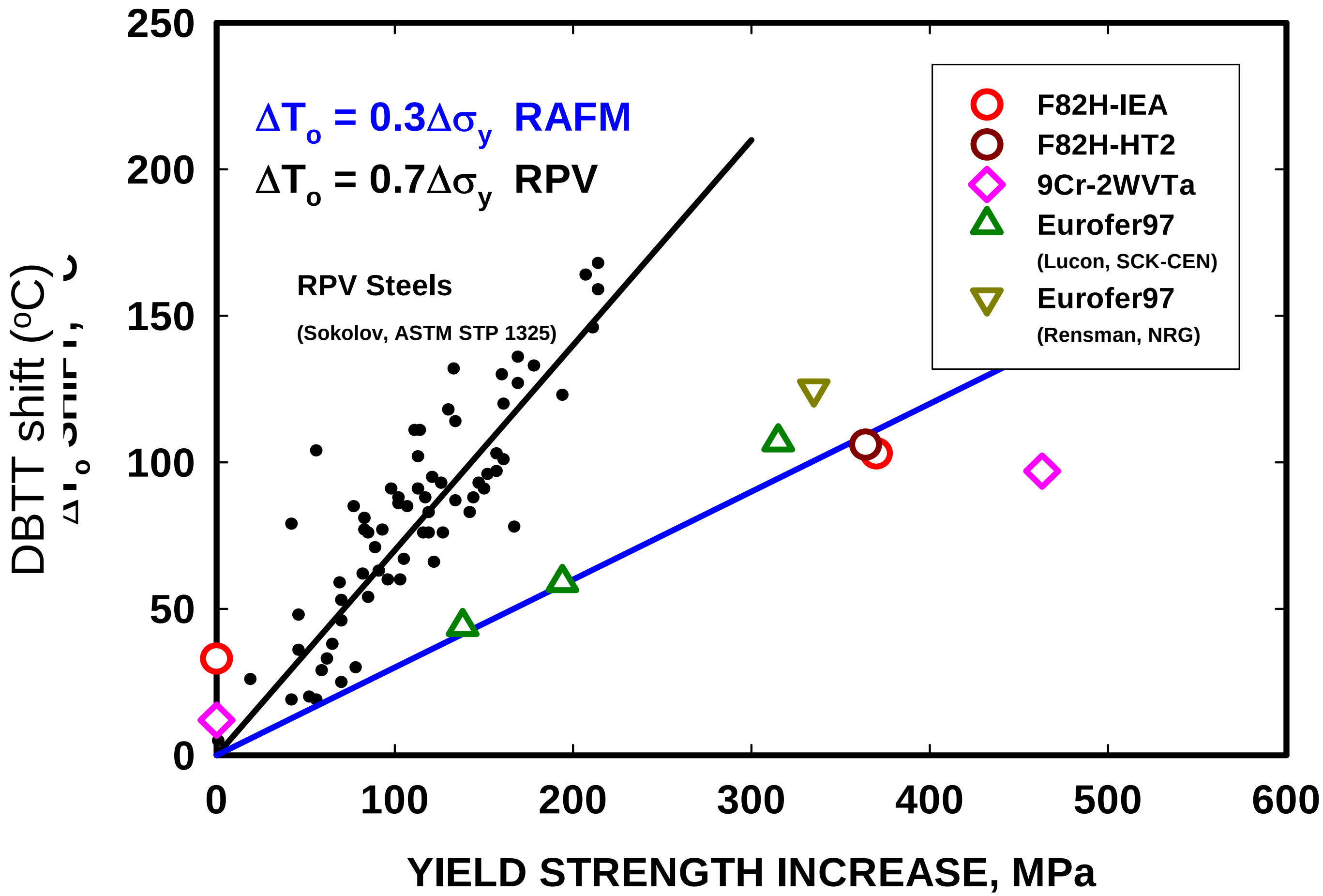




UCSB

G.R. Odette et al., J. Nucl. Mater.307-311 (2002) 171

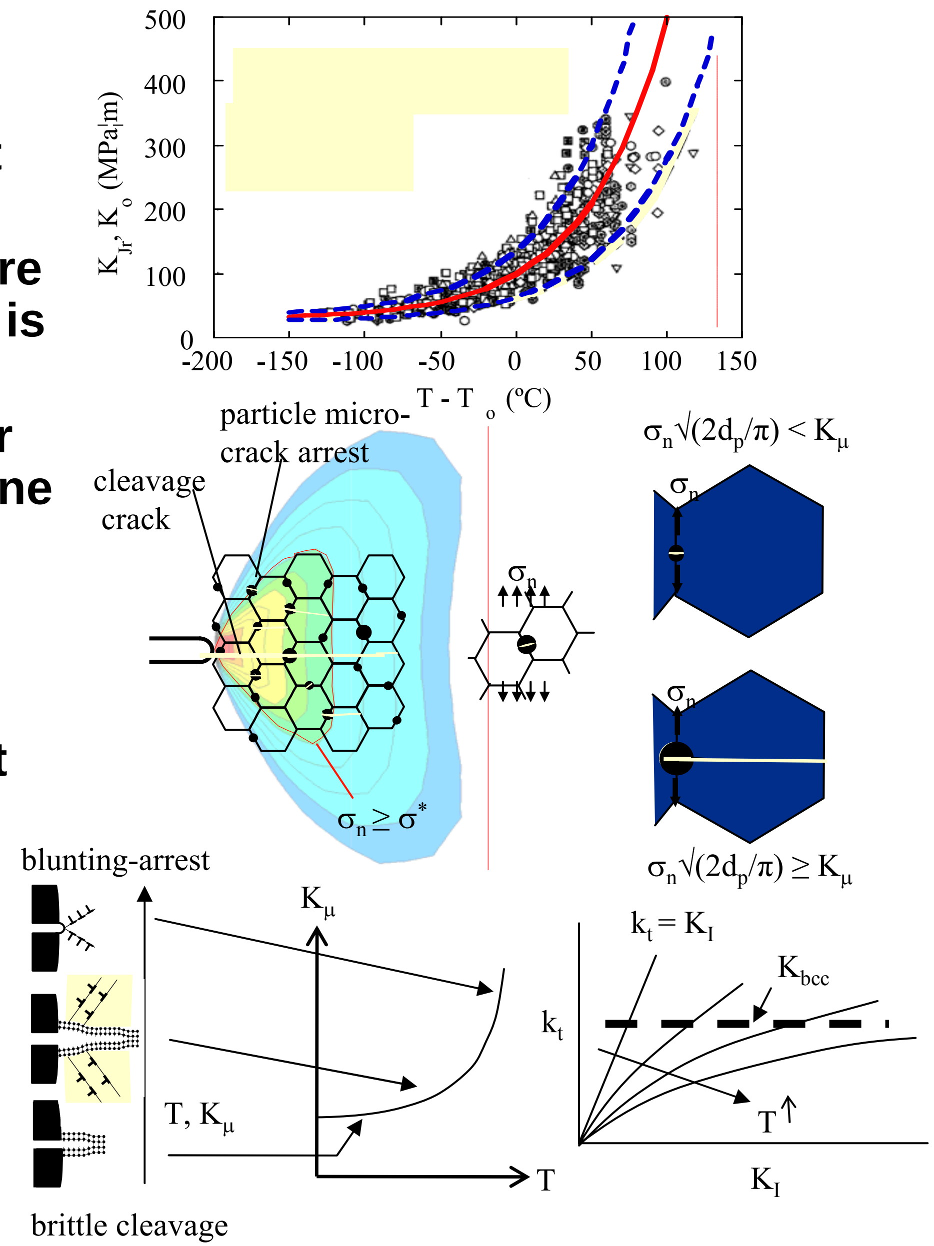
8-9%Cr RAFM Steels Exhibit Less Embrittlement Per Unit of Hardening Than Low-Alloyed RPV Steels



M.A. Sokolov et al., ICFRM12

Physical Basis for a Master Toughness Curve

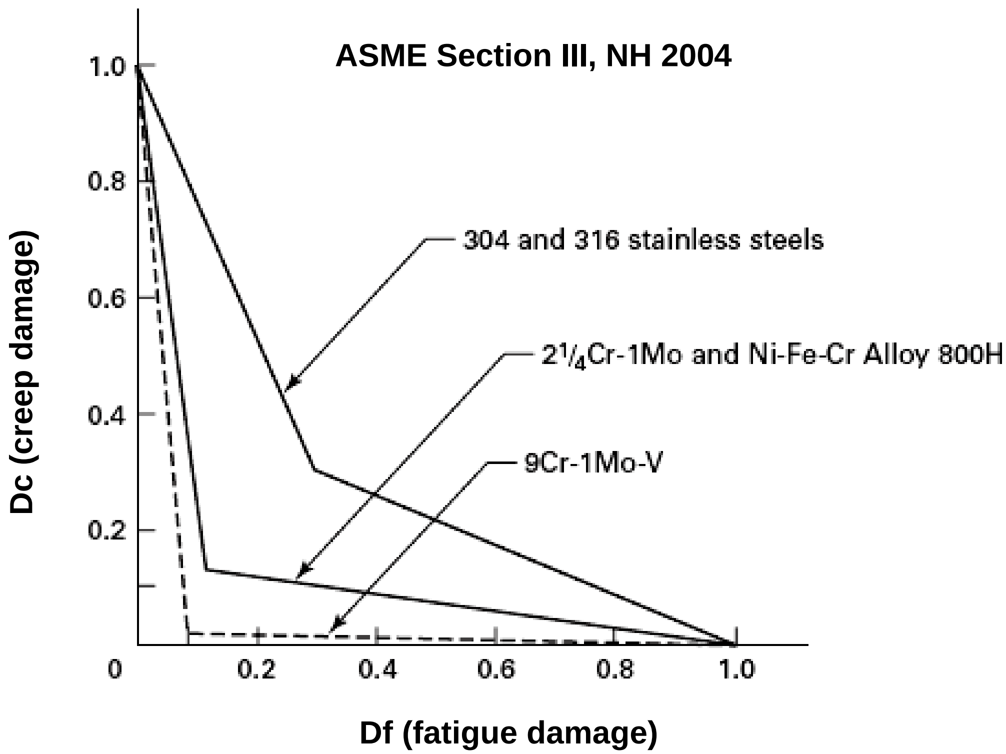
- **Master Curve method uses small specimens and ΔT models to predict fracture in large/complex structures.**
- **The universal (?) shape of the fracture toughness-temperature $K_{Jc}(T)$ curve is not understood**
- **Need integrated multiscale model for atomic scale processes that determine the macro- continuum $K_{Jc}(T)$ toughness**
- **Key? - experiments & Molecular Dynamics + Dislocation Dynamics models of intrinsic BCC micro-arrest toughness at nanoscale tip of a dynamic microcrack**



G.R. Odette, UCSB

Creep – Fatigue Interactions

- Fission reactor structural materials will experience both creep and fatigue
  - Elevated temperature design traditionally starts above 370/426°C (for steels)
    - Interaction between creep and fatigue damage not well understood
  - Large variations in creep-fatigue damage envelope exist for various materials



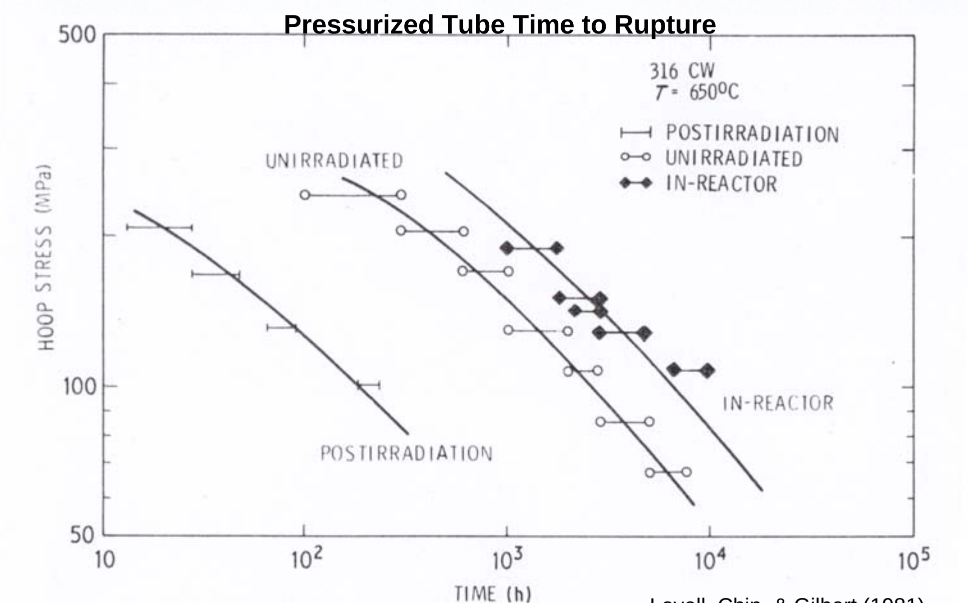
- Is linear damage rule appropriate?
- Material testing required
  - interaction mechanisms
  - damage evolution
  - cyclic wave shape & hold time
  - cold work and heat treatments
  - irradiation spectrum & dose
  - environmental effects
  - base vs. welded material
  - estimate component lifetimes
- Clear opportunities for modeling

Understanding of In-Situ Mechanical Properties Is Needed

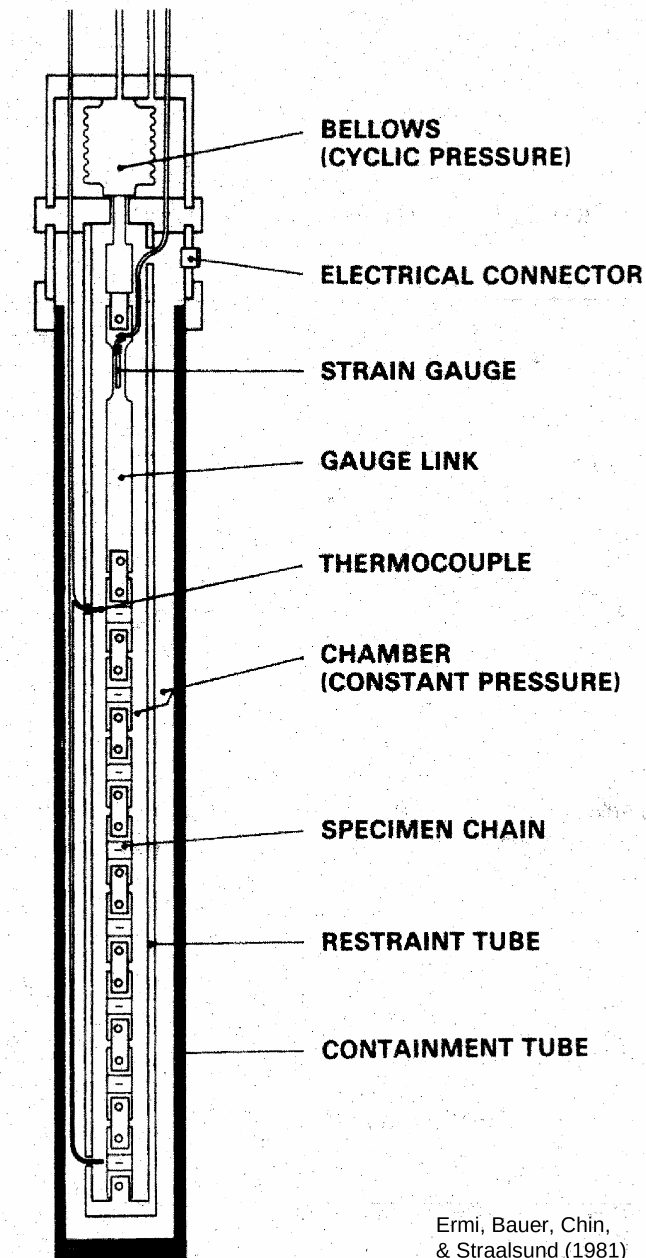
- Unknown interaction between irradiation, creep, fatigue, & swelling

- Limited in-situ tensile and creep testing has contradicted tests on post-irradiated samples (dynamic hardening, creep relaxation)

- Necessary to develop in-situ mechanical testing capabilities
  – In-reactor space requirements favor miniaturized specimens
  – Multi-specimen load trains have been demonstrated
  – Concerns of real-time deformation monitoring and consistent exposure to temperature and neutron fluence



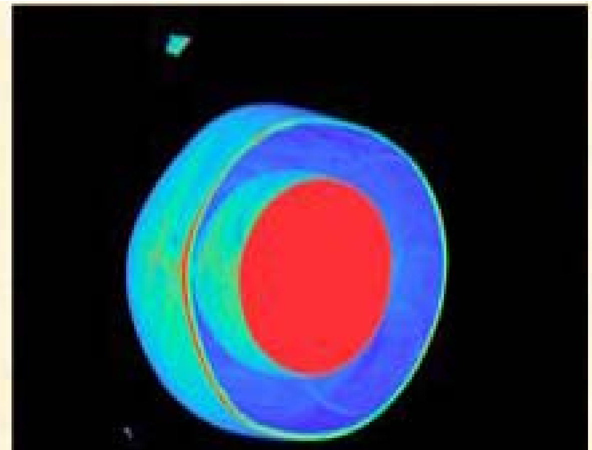
Lovell, Chin, & Gilbert (1981)



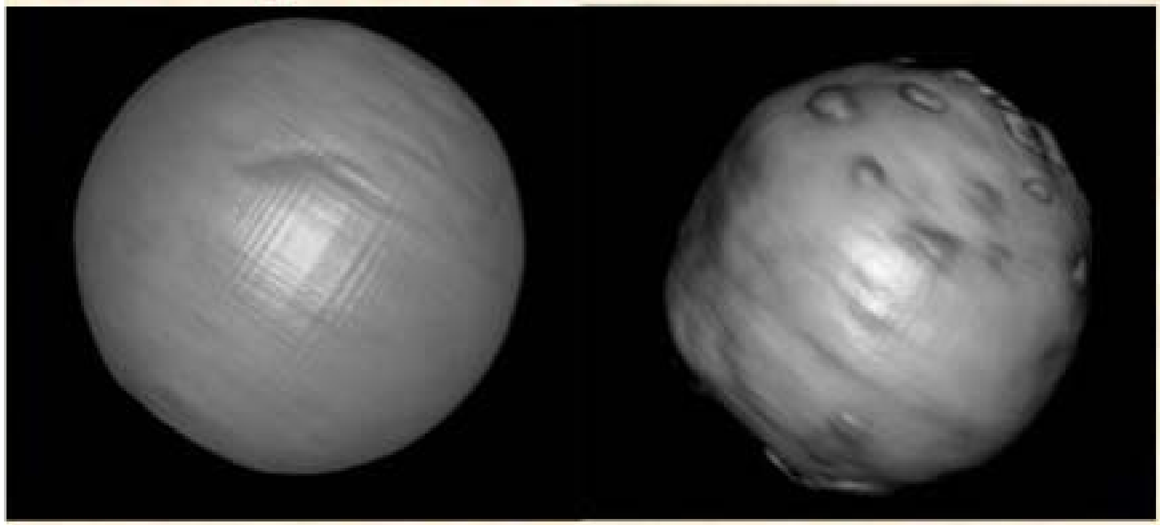
Ermi, Bauer, Chin, & Straalsund (1981)

3D X-ray tomography of TRISO fuel particles

3D renderings from tomographic data set can highlight components of a fuel particle

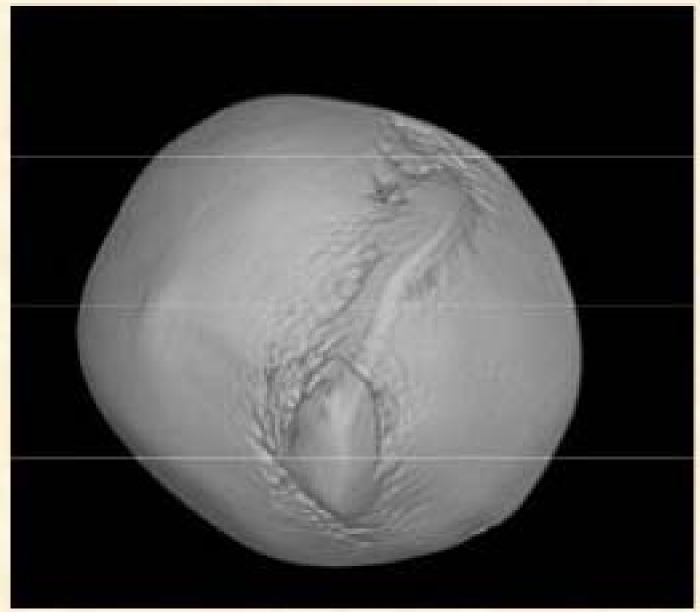


Integrity of SiC shell



Smooth (DUO_2) and bumpy (NUCO) kernels

Different materials are selected by setting a threshold value for 3D rendering



SiC coating over soot to form a "gold spot" defect

Fission Reactor Materials Modeling can Contribute to the Resolution of Several Grand Challenges in the General Field of Materials Science

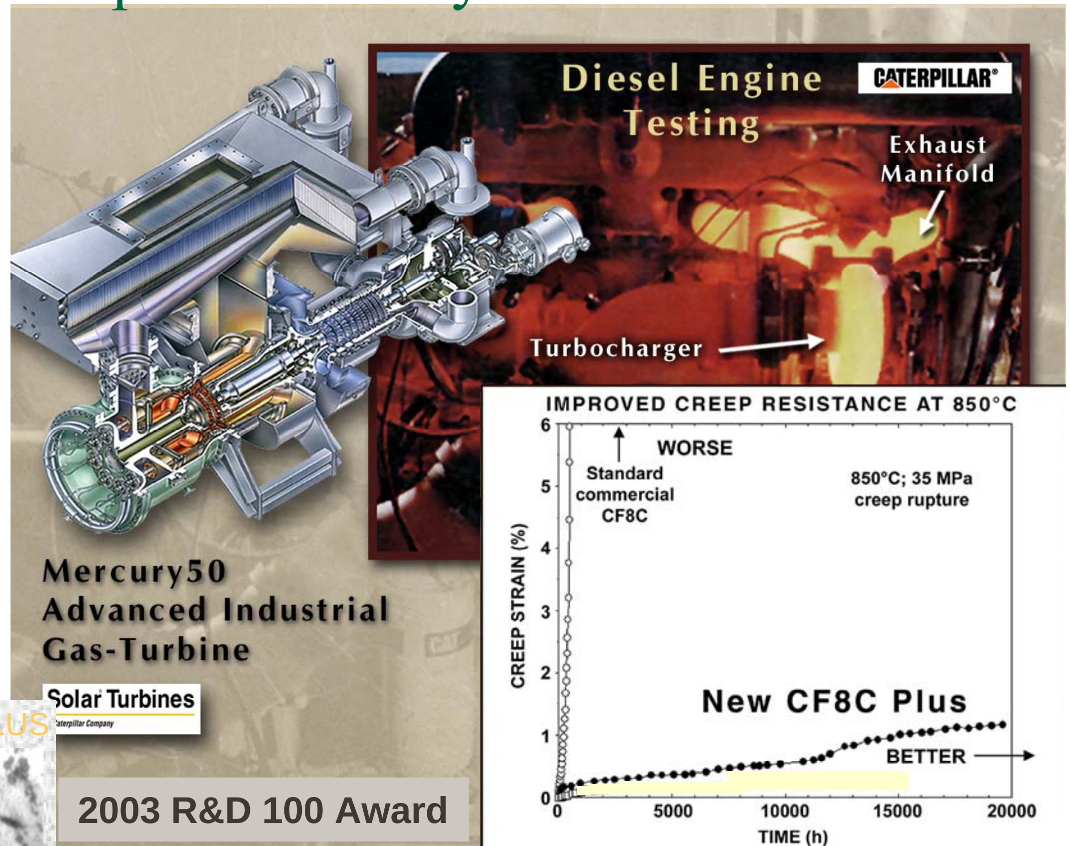
- **What are the maximum limits in strength and toughness for materials?**
  - **Dislocation propagation, interaction with matrix obstacles**
- **How are the "laws" of materials science altered under nanoscale and/or nonequilibrium conditions**
  - **Critical dimensions for dislocation multiplication**
  - **Nonequilibrium thermodynamics**
- **What is the correct physical description of electron and phonon transport and scattering in materials?**
  - **Thermal and electrical conductivity degradation due to point, line and planar defects**
- **What is the effect of crystal structure and atomic order/disorder (or noncrystallinity) on the properties of matter?**

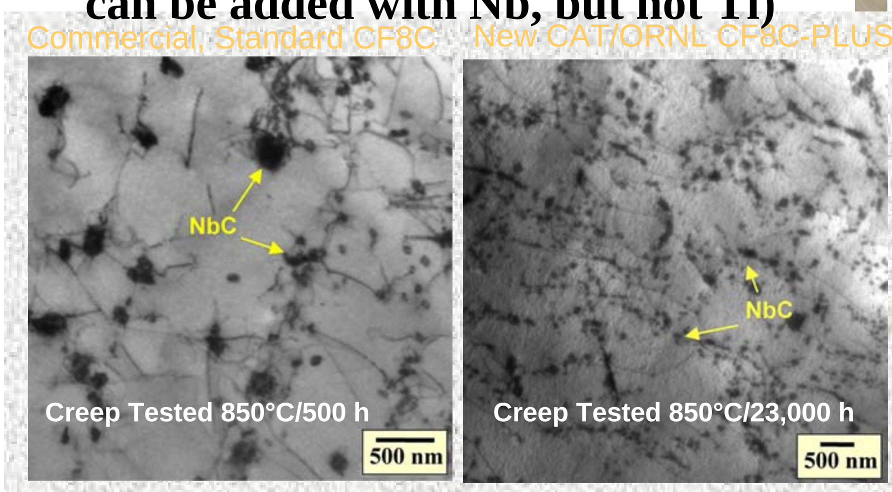
Conclusions

- Computational Materials Science offers significant benefit for accelerating the pace of development of fuels and structural materials for future nuclear energy systems
  - Numerous advanced computational tools are readily available today that were not available even 5 years ago
  - Advances in computational science are also improving the capabilities of numerous experimental validation equipment (e.g., aberation-corrected microscopes, Xray tomography)
- Validation and verification will be an essential component of a comprehensive R&D program

Microstructural Evolution In Irradiated Stainless Steels Provided the Key for Developing Improved High Temperature Alloys

- *Reactant Effects* **(ie. Ti, V+Nb enhance MC formation)**
- *Catalytic Effects* **(ie. Si enhances Fe_2Mo or M_6C)**
- *Inhibitor Effects* **(ie. C, P or B retard the formation of Fe_2Mo or FeCr sigma phase during aging, G-phase during irradiation)**
- *Interference Effects* **(ie. N forms TiN instead of TiC; N does not form NbN instead of NbC; therefore C and N can be added with Nb, but not Ti)**





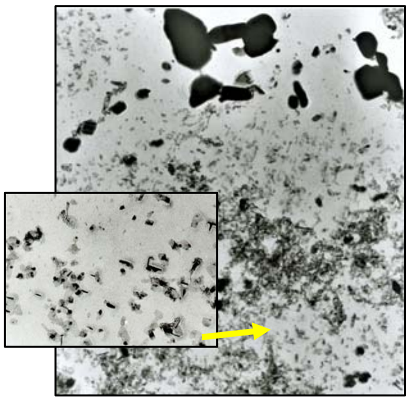
Result of microstructural modification:

- **Formation of stable nanoscale MC carbide dispersions to pin dislocations**
- **Resistance to creep cavitation and embrittling grain boundary phases (ie. sigma, Laves)**
- **Resistance to dislocation recovery/ recrystallization**

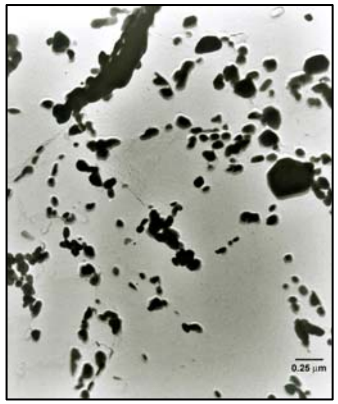
New Alloys Developed by Fusion are Being Commercialized for Advanced Manufacturing Applications: Example for 2 1/4 Cr alloys

Fusion Energy Project Led to Alloys with Exceptional Microstructure/Properties

New Microstructure Design - finer and more stable

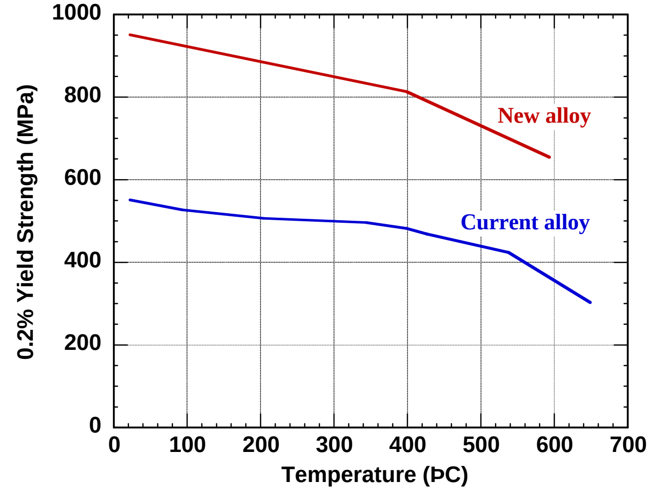


NEW: 2 1/4 Cr-2WV



Previous; 2 1/4 Cr-1Mo

Dramatic Property Improvements



1000 h creep strength is also improved by >50%

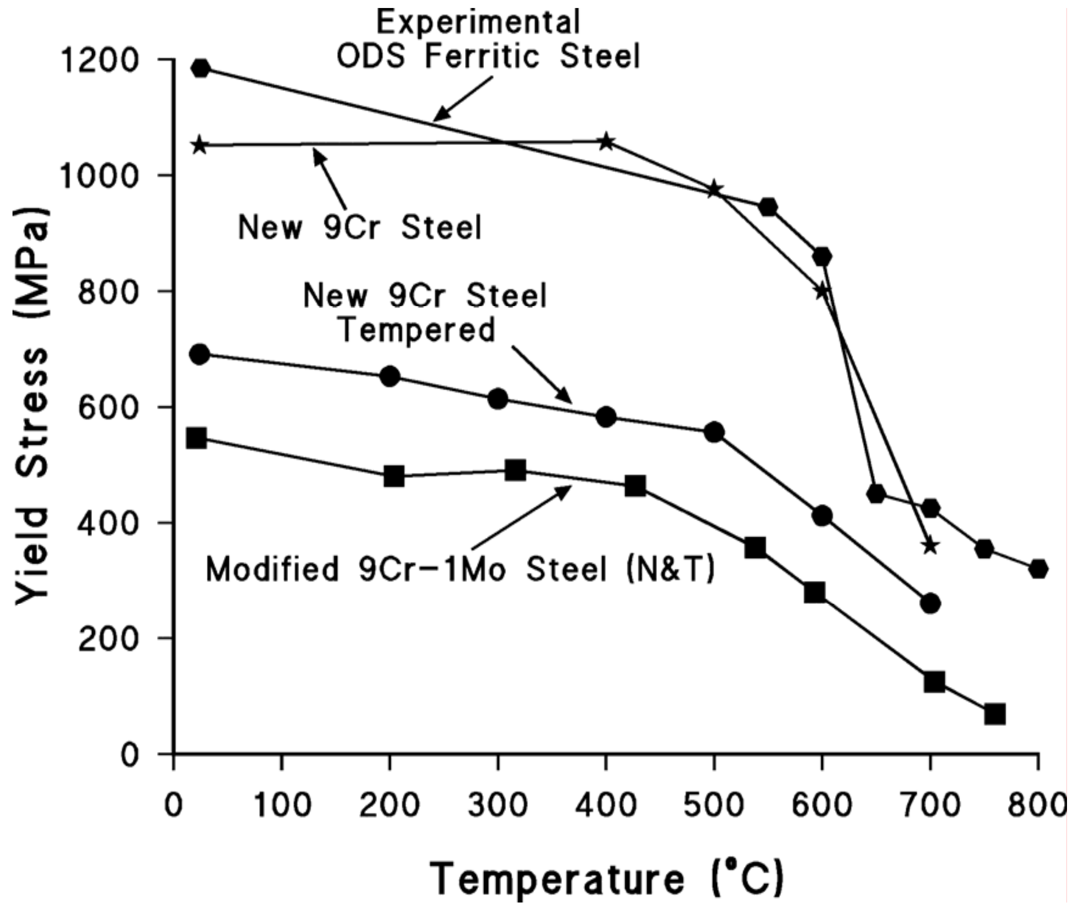
New Industrial Materials for the Future Project Focuses on Chemical Industry Applications

Planned Work:

- **Develop more advanced alloy compositions**
- **Scale up processing and fabrication**
- **Develop case-specific materials properties and welding technology**

Modified Chemistry and Thermomechanical Treatment Procedure for New 9Cr Ferritic/Martensitic Steel Produces High Strength

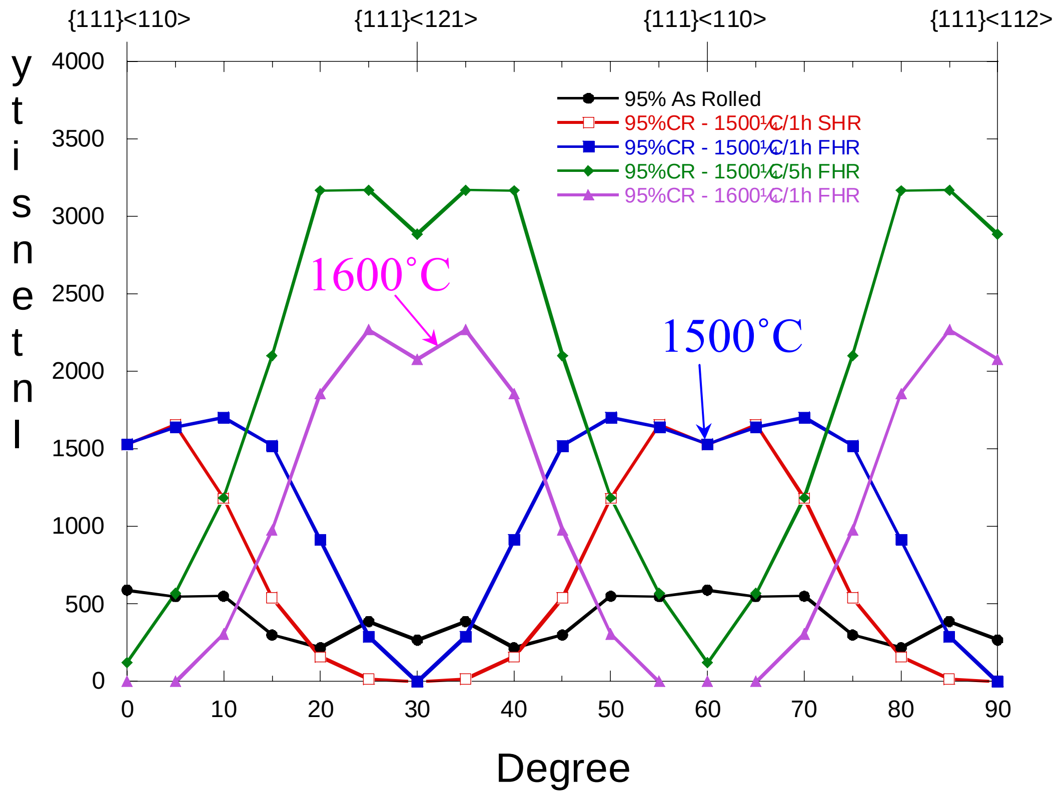
- **Strength and ductility in tensile test are comparable to high-strength experimental ODS steel**



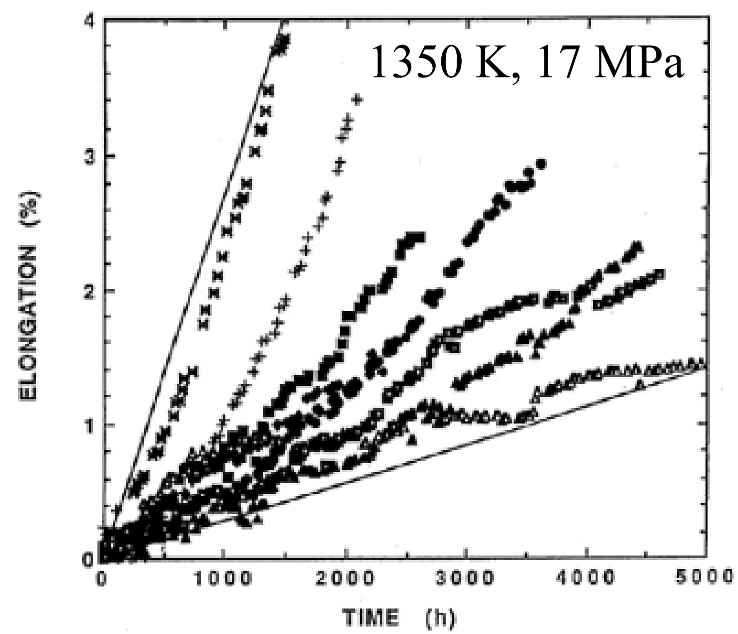
R.L. Klueh et al., Scripta Materialia (2005)

Microstructural texture may be an important contributor to the mechanical performance of materials

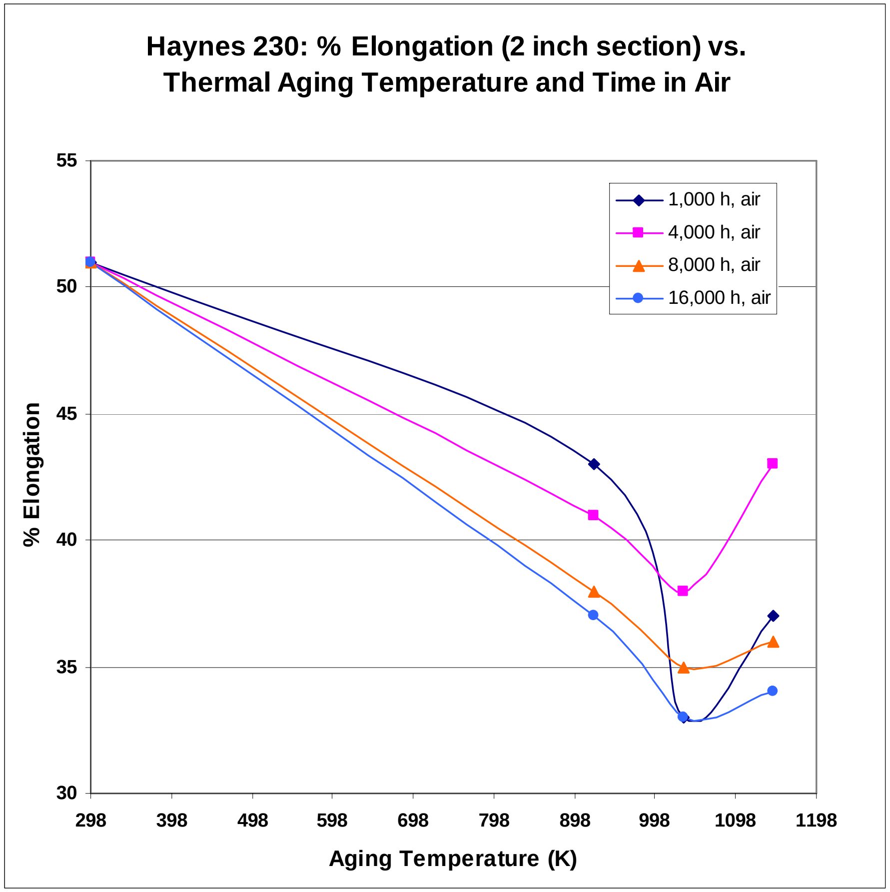
Texture in recrystallized Nb-1Zr changes dramatically between annealing temperatures of 1500 and 1600˚C

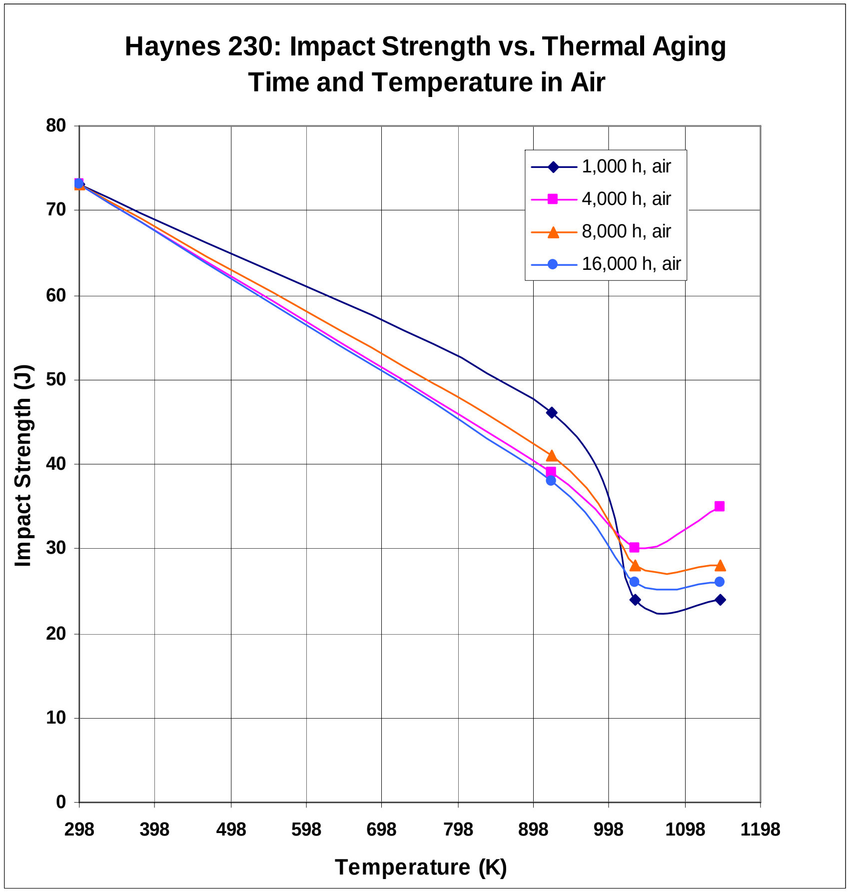


This may contribute to the observed large variability in thermal creep behavior of Nb-1Zr



Haynes 230 superalloy shows evidence of impact property degradation during aging above 900 K





Advanced Materials Characterization Tools are Needed to Examine Candidate Reactor Materials

- **Phase Analysis**
  - **Optical and electron microscopy (TEM, SEM)**
  - **Hi-temp X-ray,synchrotron, and neutron diffraction**
  - **Raman microscopy**
- **Texture**
  - **X-ray,synchrotron, and neutron diffraction**

- **Residual stress measurement**
  - **XRD, synchrotron, and neutron diffraction**
  - **Macro- and micro-stresses in two-phase mixtures**
- **Thermophysical properties**
- **Mechanical properties**
  - **Under controlled atmospheres, at elevated temp.**

(Blue color denotes activities currently available for highly radioactive materials)